3-D Computational Fluid Dynamic Modeling of the Chemical Oxygen-Iodine Laser

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Challenge Project C41

Overview

- Role of modeling activities in Air Force chemical laser program.
- Description of COIL.
- Problem Description.
- Methodology.
- Code Performance.
- Results and Progress to Date.
- Future Work.
- Summary.

Team Members

- Air Force Research Laboratory, Directed Energy Directorate, High Power Lasers Branch (AFRL/DELC).
- Logicon Company of Northrup-Grumman.
- Scientific Research Associates.
- AeroSoft, Inc.

Role of Modeling Activities at DELC

- Modeling activities at DELC contribute to the Air Force mission in multiple ways:
  - Supports Airborne Laser (ABL) development.
    - » Explain data from laser module tests and provide information beyond test diagnostics.
    - » Impact flight hardware development.
  - Enhances AFRL/DELC experiment activities:
    - » Provides insight into the physical processes underlying the experiment.
    - » Predicts quantities not measured by experiment diagnostics.
    - » Designing new experiments.
    - » Helps identify and evaluate new research pathways.
- The goal of the modeling effort is not to simply match experiment data *but to explain the data*.

What is a COIL?

- The Chemical Oxygen-Iodine Laser is a laser that uses the electronic state transition of the iodine atom:

$$I(^2P_{1/2}) \rightarrow I(^2P_{3/2}) + h\nu$$

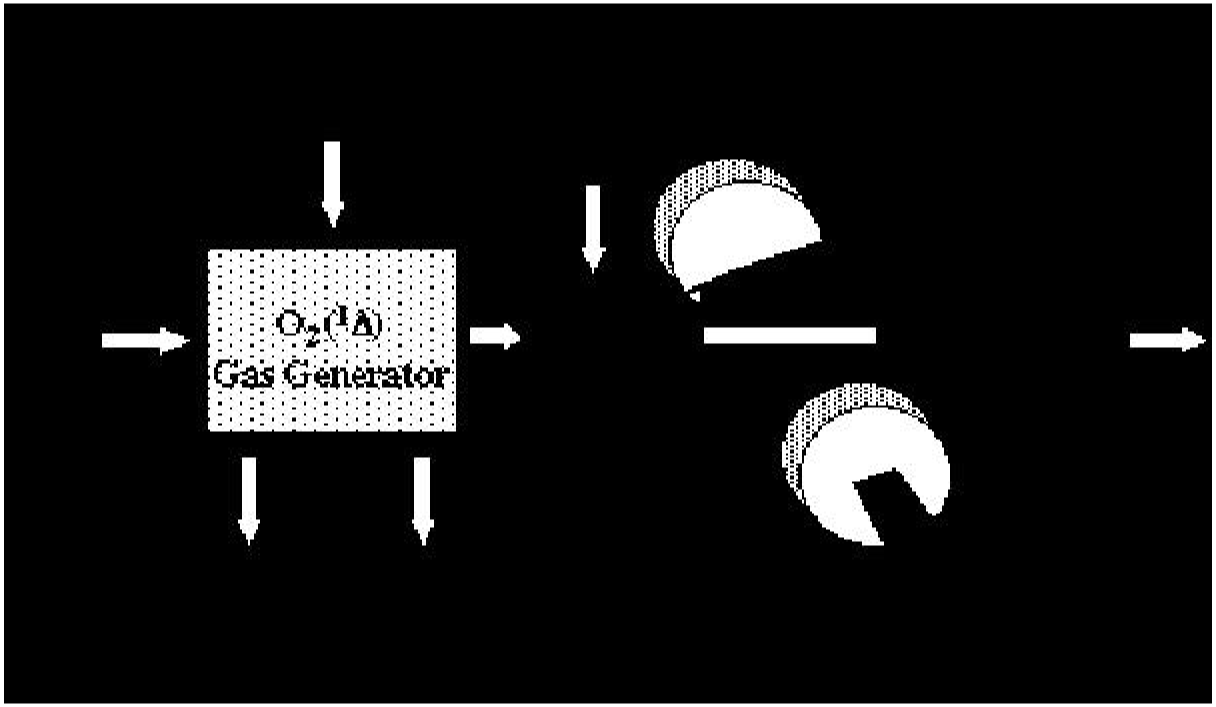
$$I(^2P_{1/2}) + h\nu \rightarrow I(^2P_{3/2}) + 2h\nu$$

to produce photons with a wavelength of 1.315 μm.

- Before $I(^2P_{1/2})$ appears, a complex series of processes in the COIL must occur:
  - Produce $O_2(^1\Delta)$
    - » $Cl_2 + 2HO_2^- \rightarrow O_2(^1\Delta) + H_2O_2 + 2Cl$
  - Produce I atoms from I_2
    - » $O_2(^1\Delta) + I_2 \rightarrow O_2(^3\Sigma) + I_2^*$
    - » $O_2(^1\Delta) + I_2^* \rightarrow O_2(^3\Sigma) + 2I(^2P_{3/2})$
  - Produce $I(^2P_{1/2})$
    - » $O_2(^1\Delta) + I(^2P_{3/2}) \rightarrow O_2(^3\Sigma) + I(^2P_{1/2})$

What is a COIL?

Diagram of the operation of a COIL.



Problem Description

- The 'typical' Challenge class modeling problem is to mathematically describe the 3-D, chemically reacting, photon emitting, viscous flow within chemical lasers.
  - The resulting set of nonlinear partial differential equations (pde's) are beyond analytical solution and require numerical integration.
  - These equations are closely coupled at the timescales of the dominant physical processes, yet contain descriptions of processes that may vary across a wide range of timescales.
  - The physical domain in which the equations must be integrated is usually geometrically complex.
  - Simulation using numerical integration of this system requires solution techniques capable of accurately integrating the equations while maintaining numerical stability.

Solution Methodology

- Integrate the full, laminar 3-D Navier-Stokes equations coupled to continuity equations for the species components of the flow.
- Thermo-chemistry, multi-component molecular diffusion, and power extraction models particular to chemical laser analysis have been added to the codes.
- Both models in use at DELC are built upon commercial computational fluid dynamic (CFD) codes.
  - MINT from Scientific Research Associates
  - GASP from AeroSoft, Inc.

GASP

- Conservative finite volume formulation of the Navier-Stokes and species continuity equations.
- 3rd order, upwind-biased differencing of spatial derivatives.
- 1st order Euler implicit time integration.
- Jacobi inner iteration solution of matrices generated for implicit time integration.
- Finite rate chemistry modeling.
- Conservative, multi-component diffusion modeling.
- Domain decomposition into coupled zones for multi-processor execution.
  – OpenMP message passing protocol used, limited to shared memory execution at this time.
- Extensively validated for a variety of external and internal flow problems.

MINT

- Conservative finite difference formulation of the Navier-Stokes and species continuity equations.
- 2^{nd} order, central differencing of spatial derivatives.
- 2^{nd} order Euler implicit time integration.
- Alternating Direction Implicit (ADI) solution of implicit time integration matrices.
- Finite rate chemistry modeling.
- Conservative, multi-component diffusion modeling.
- Geometric optics power extraction model.
- H_2O condensation and H_2O particle tracking.
- Outer loop parallelization of ADI scheme using MPI message passing protocol for multi-processor execution.

Multicomponent Molecular Diffusion Model

- Effective diffusion model used to compute diffusive fluxes important at low Reynolds numbers.

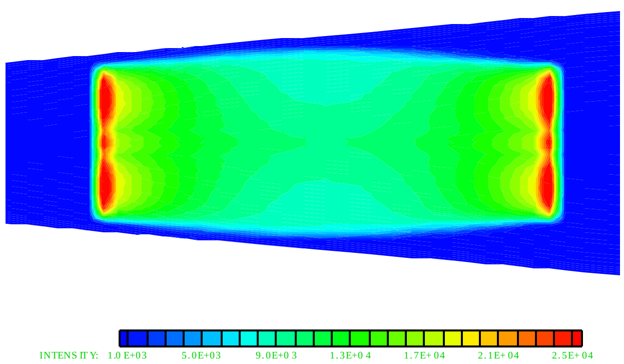
$$r_i \vec{v}_i = -n m_i D_{im} \left[\frac{\P c_i}{\P \vec{r}} + \left(c_i - f_i \right) \frac{\P \ln P}{\P \vec{r}} \right]$$

$$+ \mathrm{f}_{\mathrm{i}} n \sum_{j=1}^{N} m_j D_{jm} \left[\frac{\P c_j}{\P \vec{r}} + \left(c_j - f_j \right) \frac{\P \ln P}{\P \vec{r}} \right]$$

$$D_{im} = \frac{\left(1 - c_i\right)}{\displaystyle\sum_{j=1,\, j \neq i}^{N} \frac{c_j}{D_{ij}}}$$

Stable Resonator Model for Power Extraction

- Geometric optics stable resonator model solves ray trace equations.
  - Iterates intensity field with the gain field until round trip gain equal loss conditions satisified.
  - Mirror geometry consists of flat outcoupler and hemispherical reflector for specified reflectivities and losses.
  - Diffraction incorporated via input aperture loss.



MINT Stable Resonator Output

Gain Model

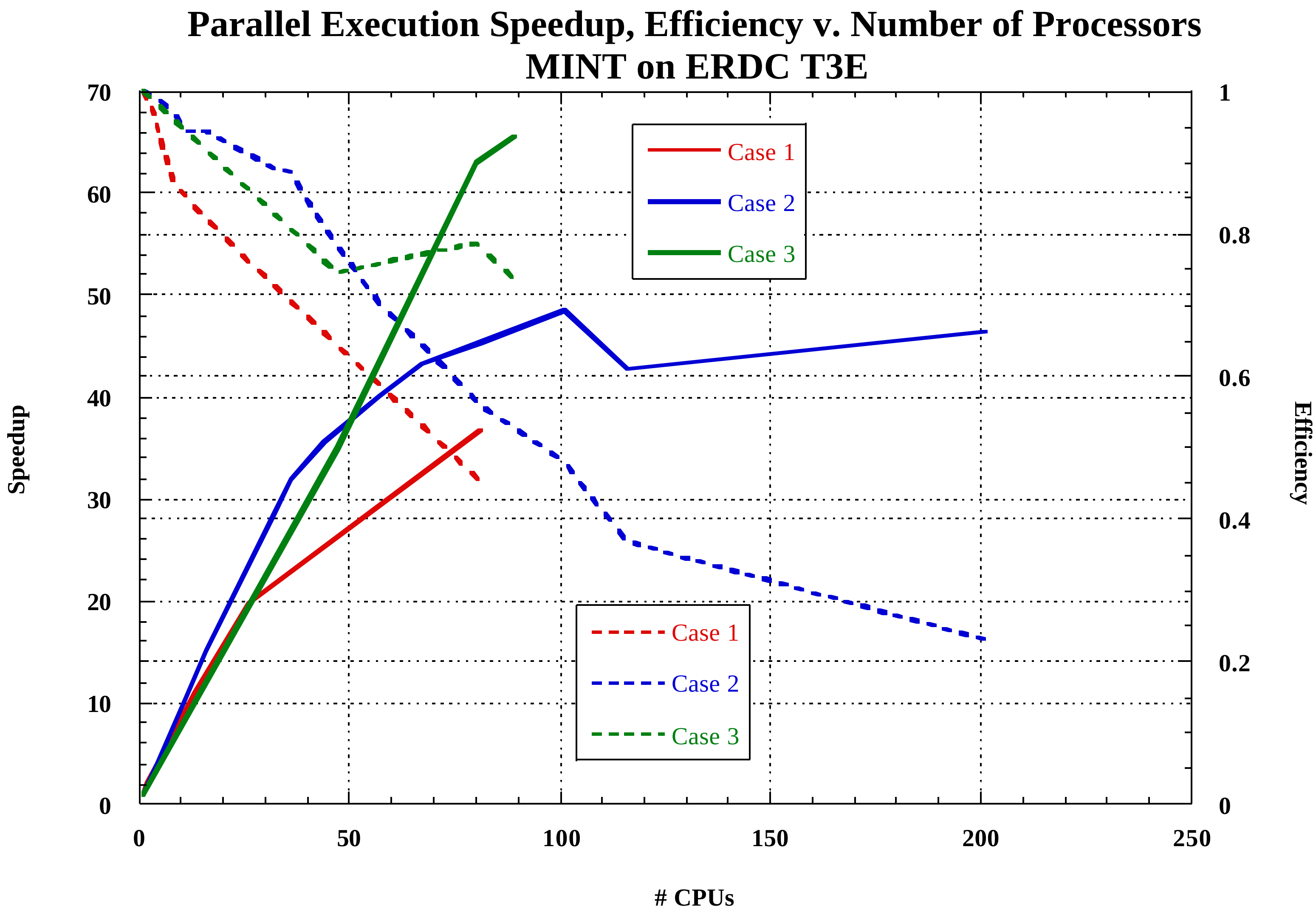
- Gain expression for I($^2P_{1/2}$) to I($^2P_{3/2}$) transition.

$$gain = \frac{7}{12}\left(\frac{A\lambda^2}{8\pi}\right) f(\nu)\left(N_{I(^2P_{1/2})} - \frac{1}{2}N_{I(^2P_{3/2})}\right)$$

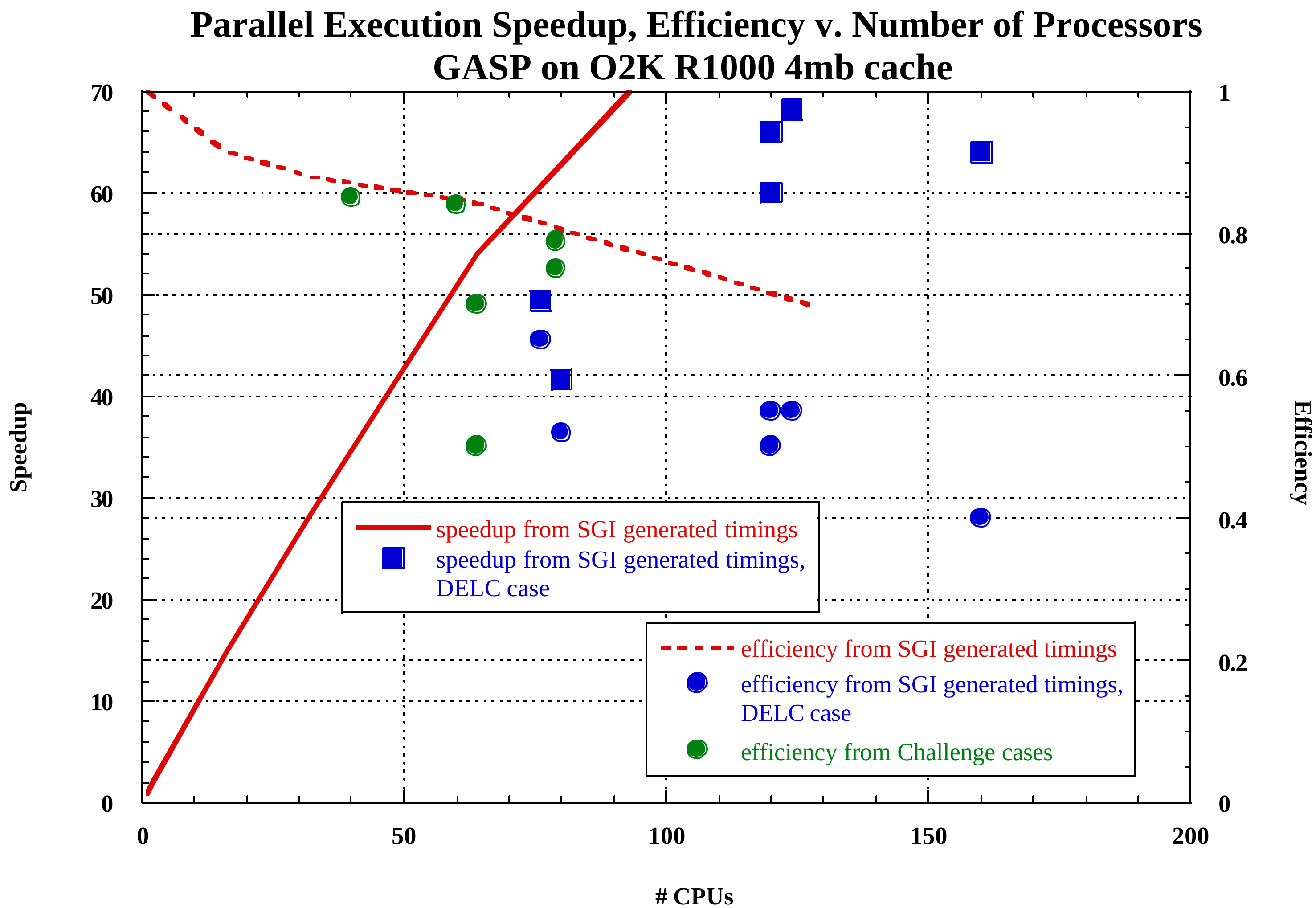
$$f(\nu) = \frac{2}{\Delta\nu_D}\left(\frac{\ell n2}{\pi}\right)^{1/2}\left[1 - erf\left\{\frac{\Delta\nu_L}{\Delta\nu_D}\sqrt{\ell n2}\right\}\right]\exp\left(\left\{\frac{\Delta\nu_L}{\Delta\nu_D}\sqrt{\ell n2}\right\}^2\right)$$

$$\Delta\nu_D = \frac{2}{\lambda}\sqrt{\frac{2RT\ell n2}{m_I}} \qquad \Delta\nu_L = \frac{T_{ref}}{T} P\sum_{i=1}^{N}\alpha_i c_i$$

Parallel Scaling Performance



Parallel Scaling Performance



Current Challenge Work

- Current efforts:
  - Support ABL through 3-D simulation of the full laser module (FLM).
    - » Simulate supersonic recovery region.
    - » Develop ‘end to end’ 3-D model for the FLM.
      - Simulate FLM tests to baseline the model.
      - Use this model to ‘extend’ the FLM database beyond test diagnostic data and extrapolate to run conditions not tested.
  - Re-evaluate the Standard COIL Rate Package using the 3-D models.
    - » COIL rate package originally developed in 1987 using low order methods in comparison to the present modeling capability.
    - » Determine the sensitivity of the 3-D model predictions to the measured reaction rates that are input to the model.
    - » Use these sensitivities to recommend new reaction rate measurements.

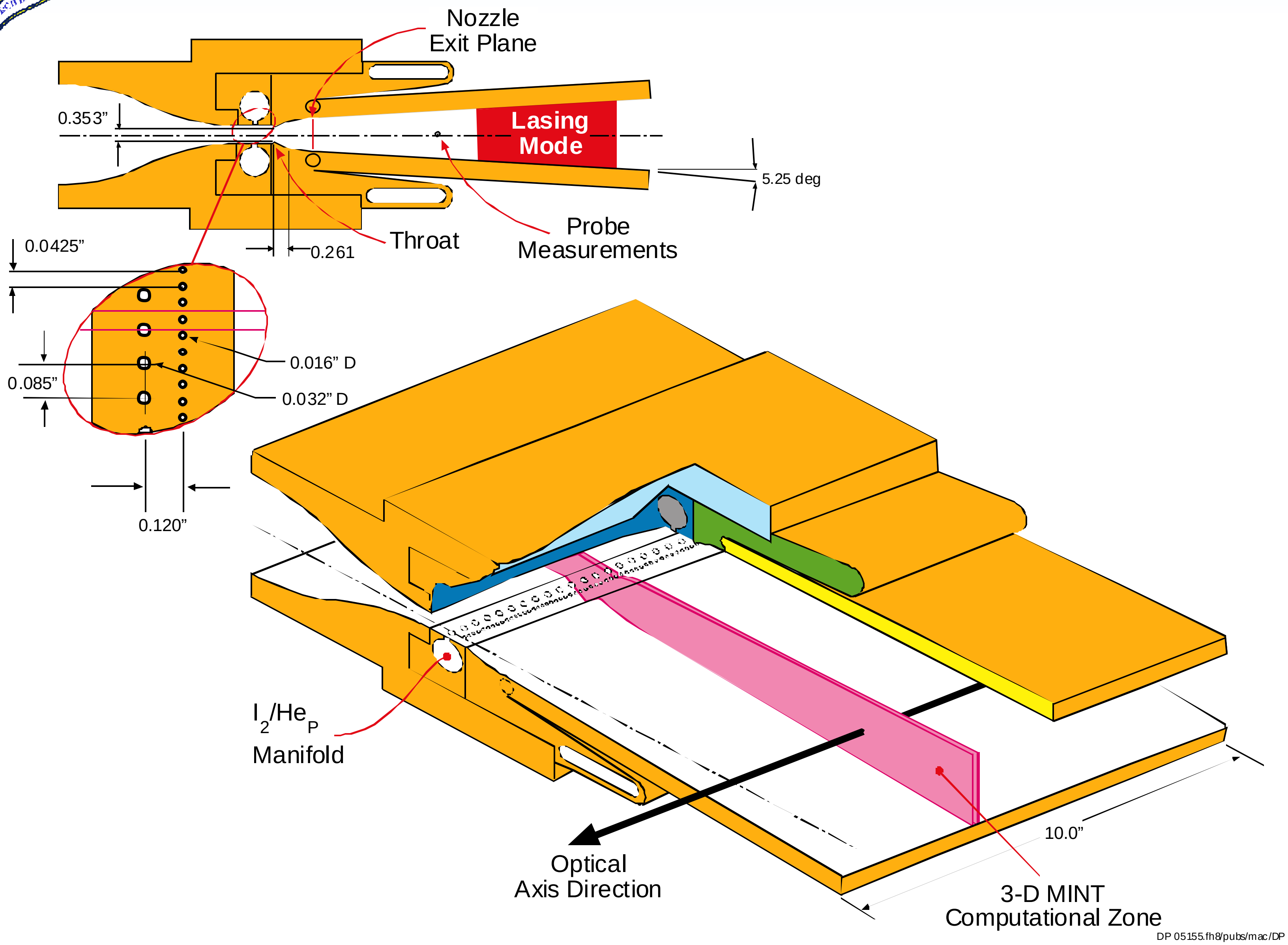
Current Challenge Work

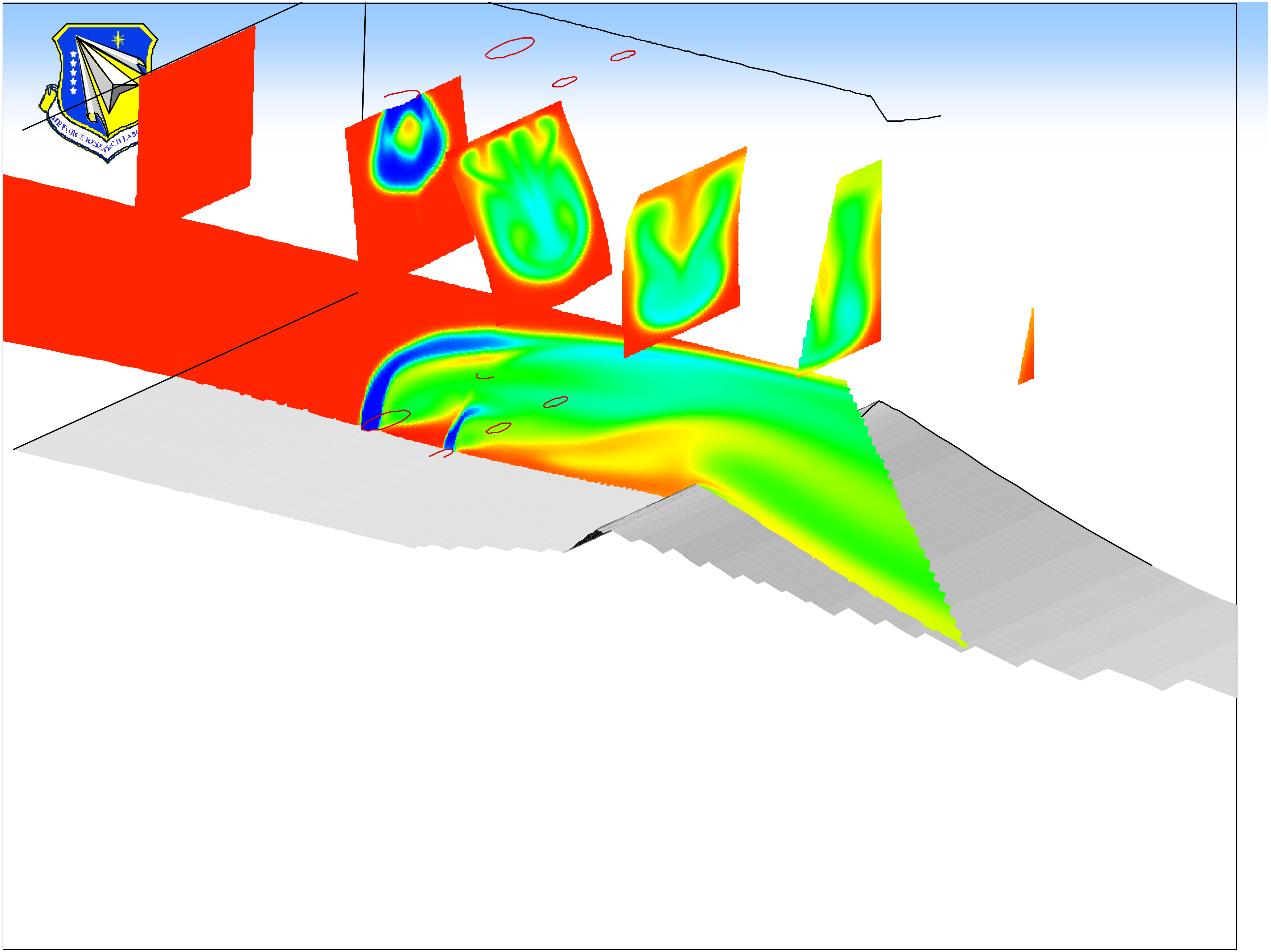
- Current Efforts:
  - Support development of the recently demonstrated all gas phase iodine laser (AGIL).
    - » AGIL generates $I(^2P_{1/2})$ via energy transfer from $NCl(a^1\Delta)$, a product of a series of all gas phase chemical reactions.
      - Important to the Air Force mission because of potential weight savings with respect to COIL.
    - » Inefficient mixing of reactants has been identified as limiting system performance in current hardware.
    - » 3-D CFD simulation is being used to examine the mixing issues and indicate hardware modifications to alleviate the problem.

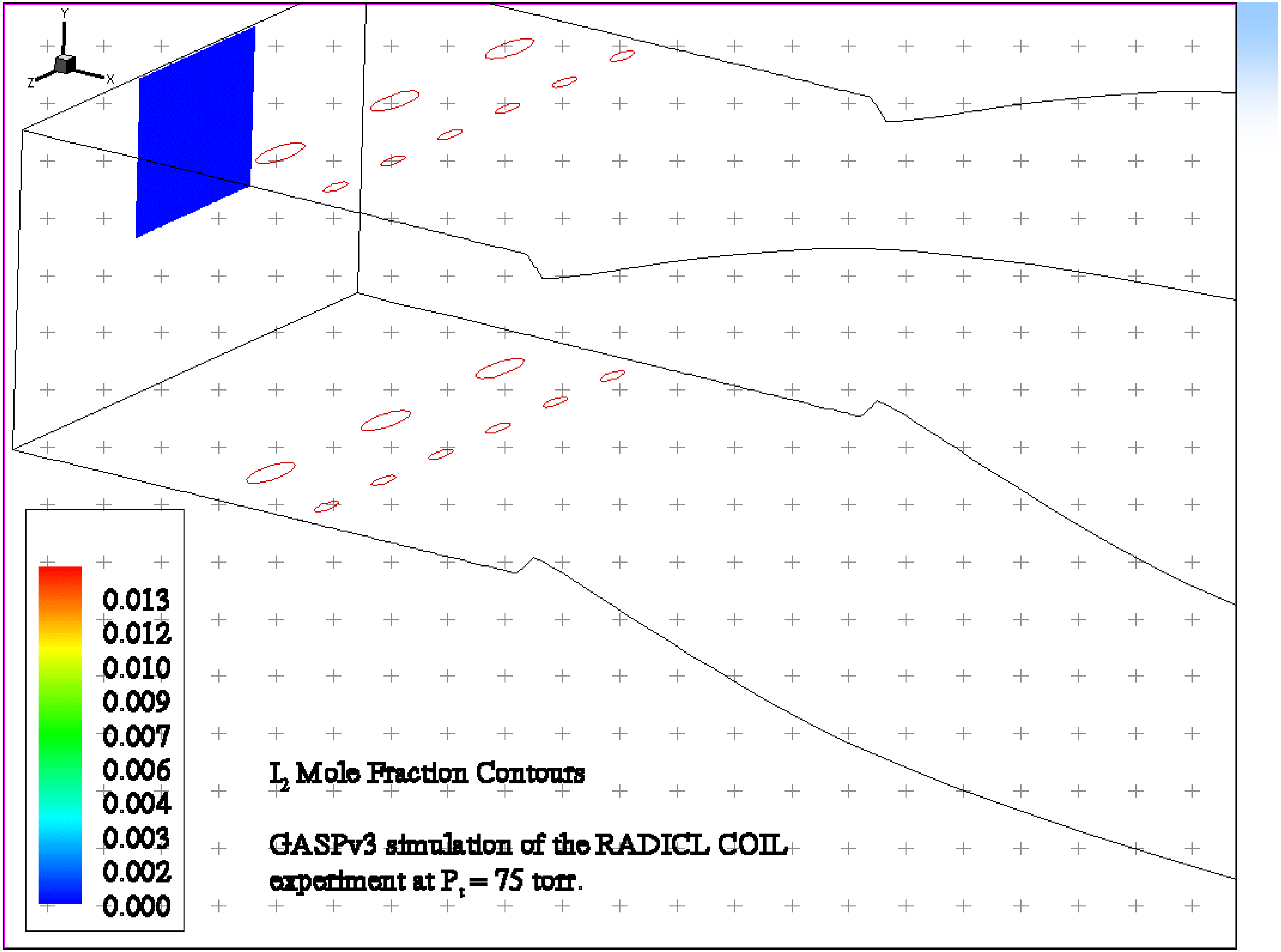
Results

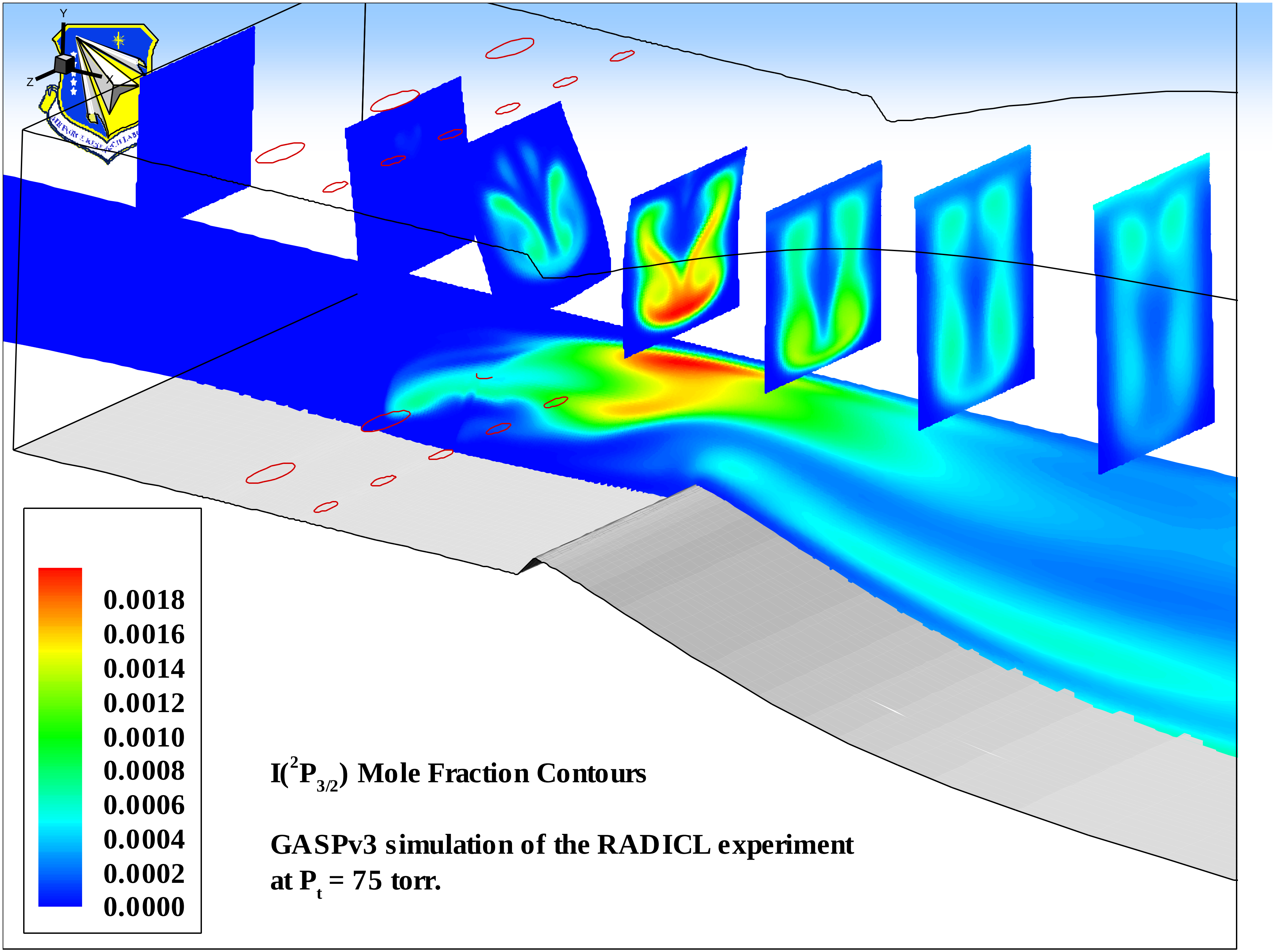
- MINT simulation of ABL FLM supersonic diffuser.
- GASP simulation of RADICL experiment used to perform COIL chemistry sensitivity analysis.
- GASP simulation of AGIL experiment hardware to help identify mixing issues.

RADICL Experiment Slit Nozzle






Y
Z
X
0.013
0.012
0.010
0.009
0.007
0.006
0.004
0.003
0.002
0.000
I_2 Mole Fraction Contours
GASPv3 simulation of the RADICL COIL experiment at $P_t = 75$ torr.


Y
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X
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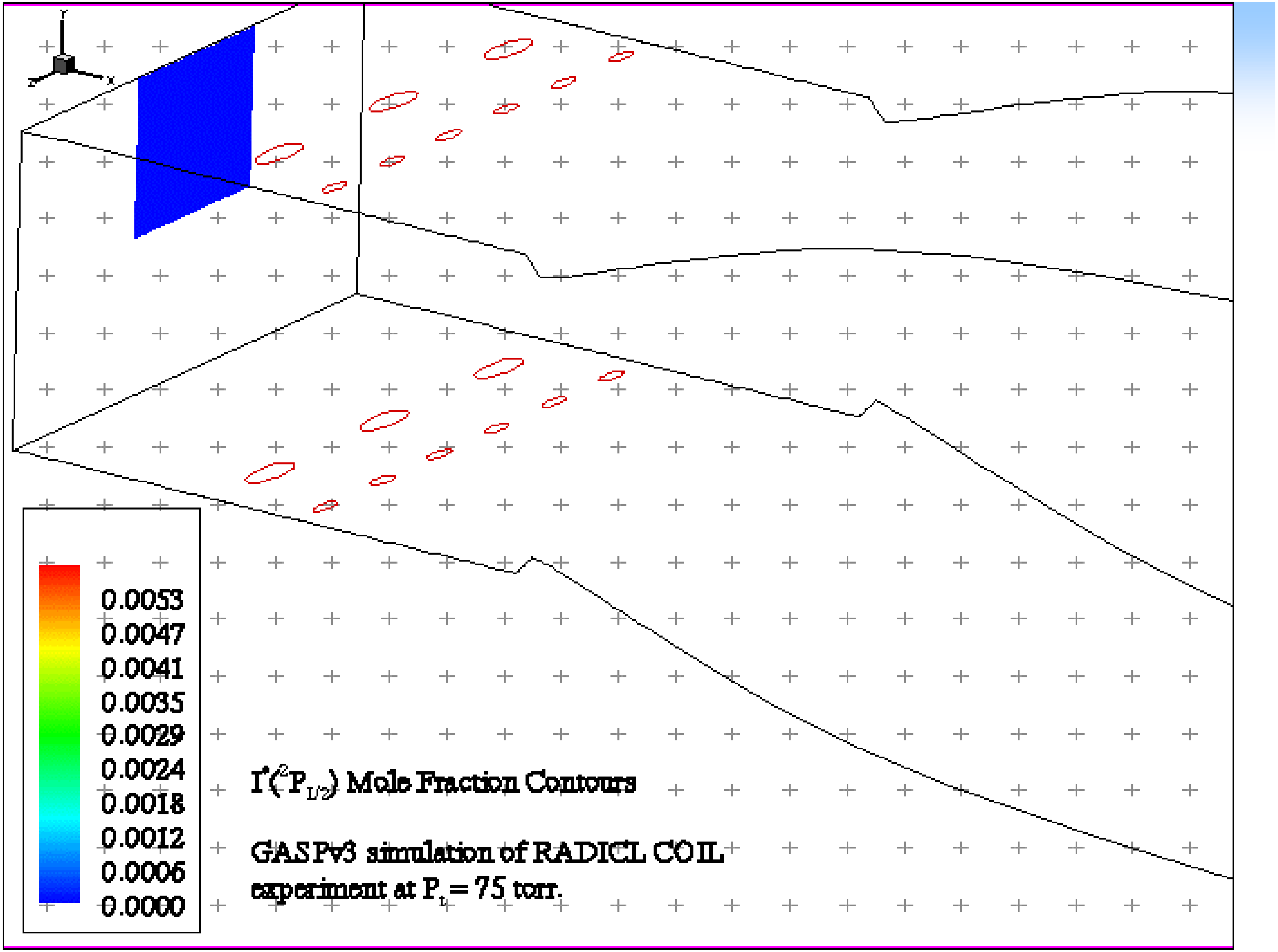
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
I($^2P_{3/2}$) Mole Fraction Contours
GASPv3 simulation of the RADICL experiment
at P_t = 75 torr.


0.0053
0.0047
0.0041
0.0035
0.0029
0.0024
0.0018
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0.0006
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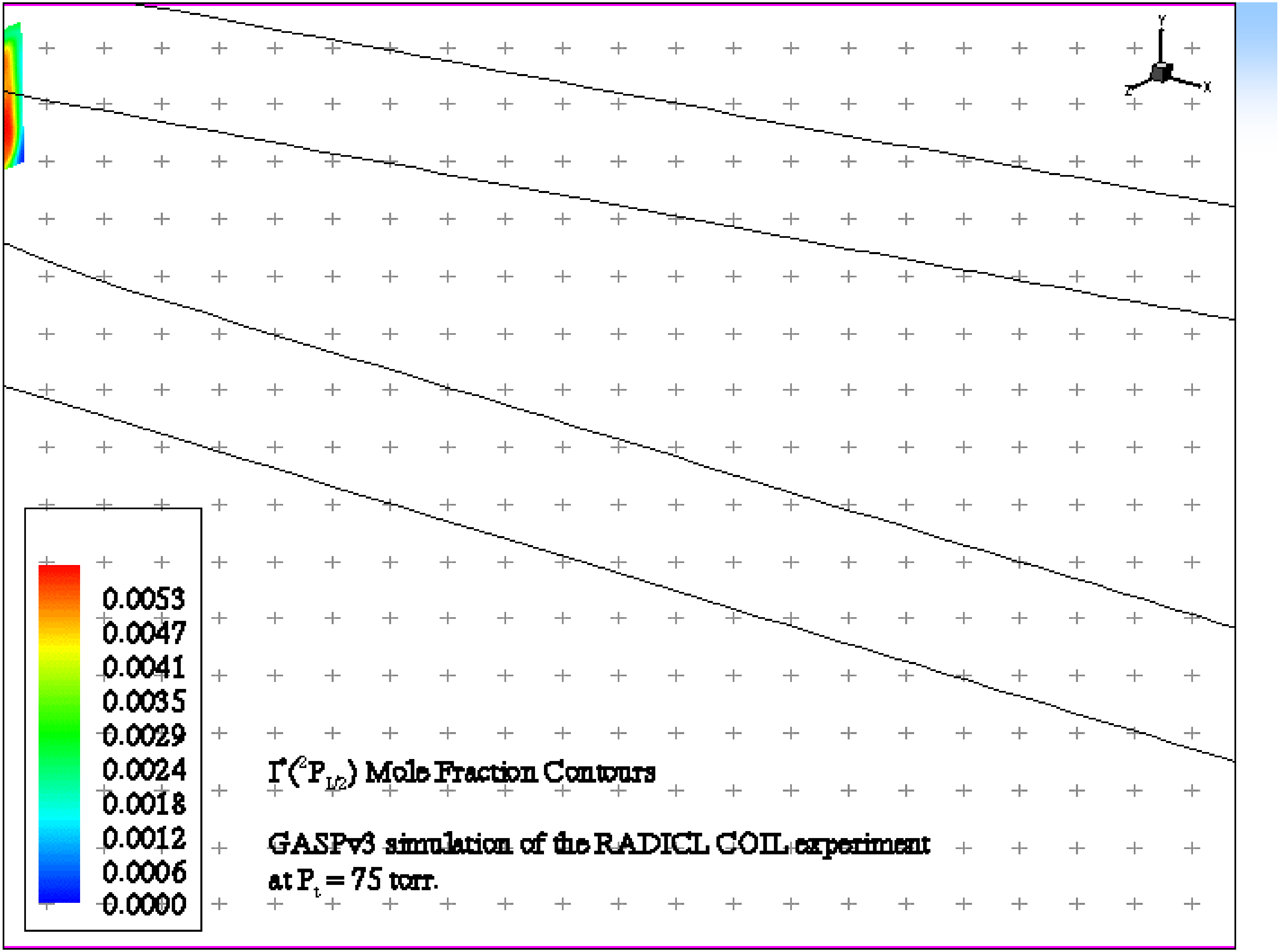
I*(²P1/2) Mole Fraction Contours
GASPv3 simulation of RADICL COIL
experiment at Pt = 75 torr.



Y
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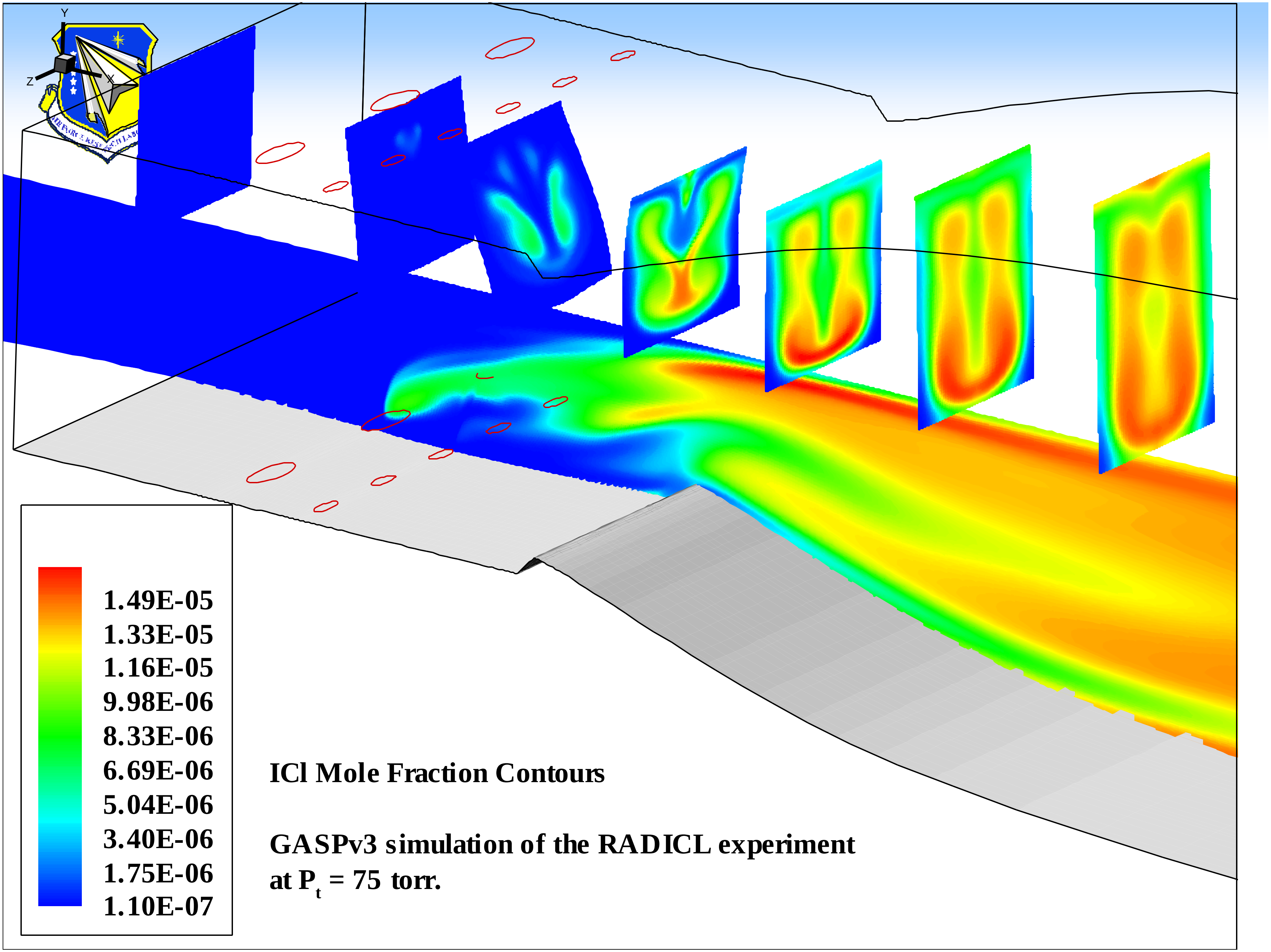
$I^*(^2P_{1/2})$ Mole Fraction Contours
GASPv3 simulation of the RADICL COIL experiment
at P_t = 75 torr.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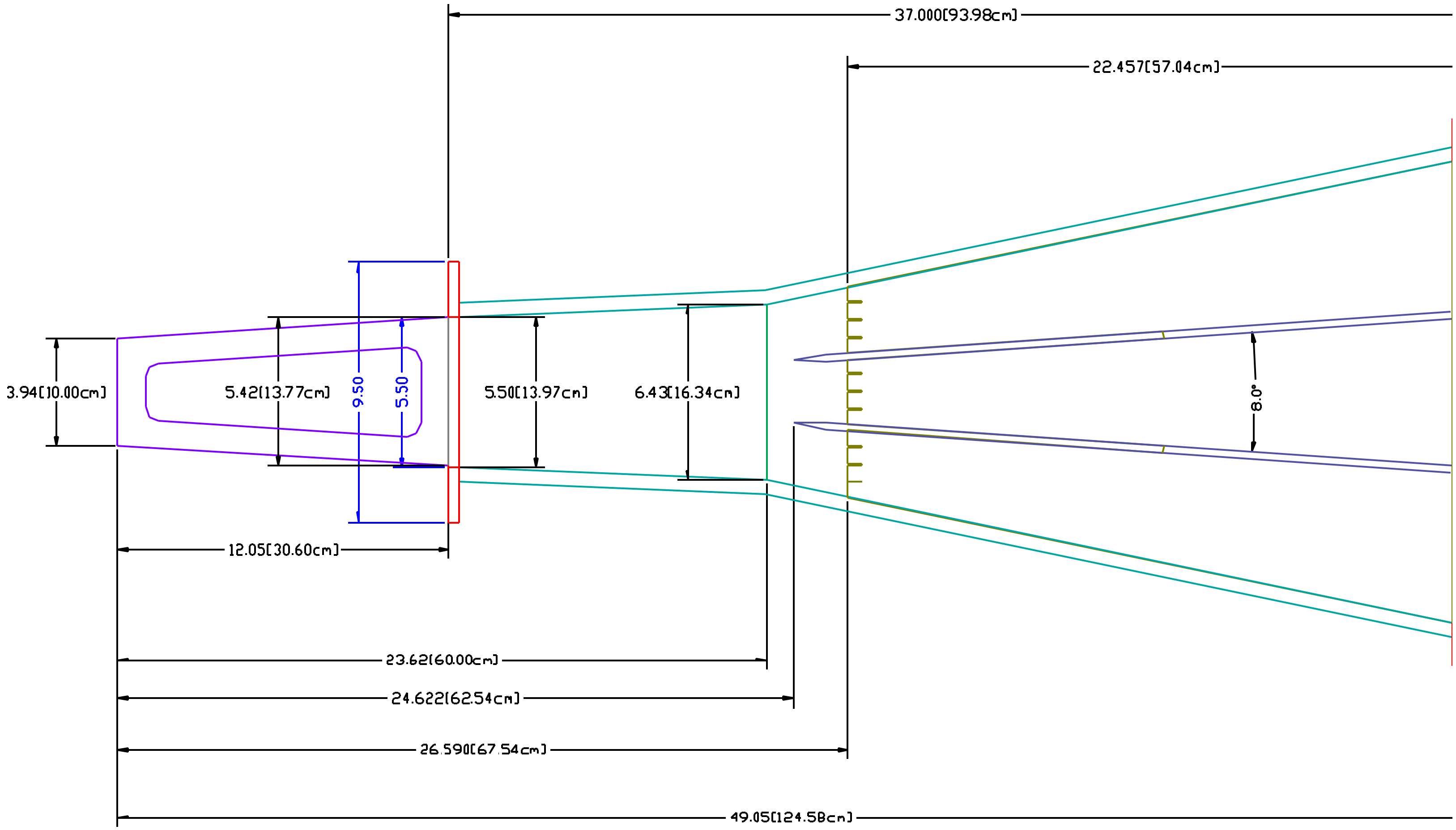
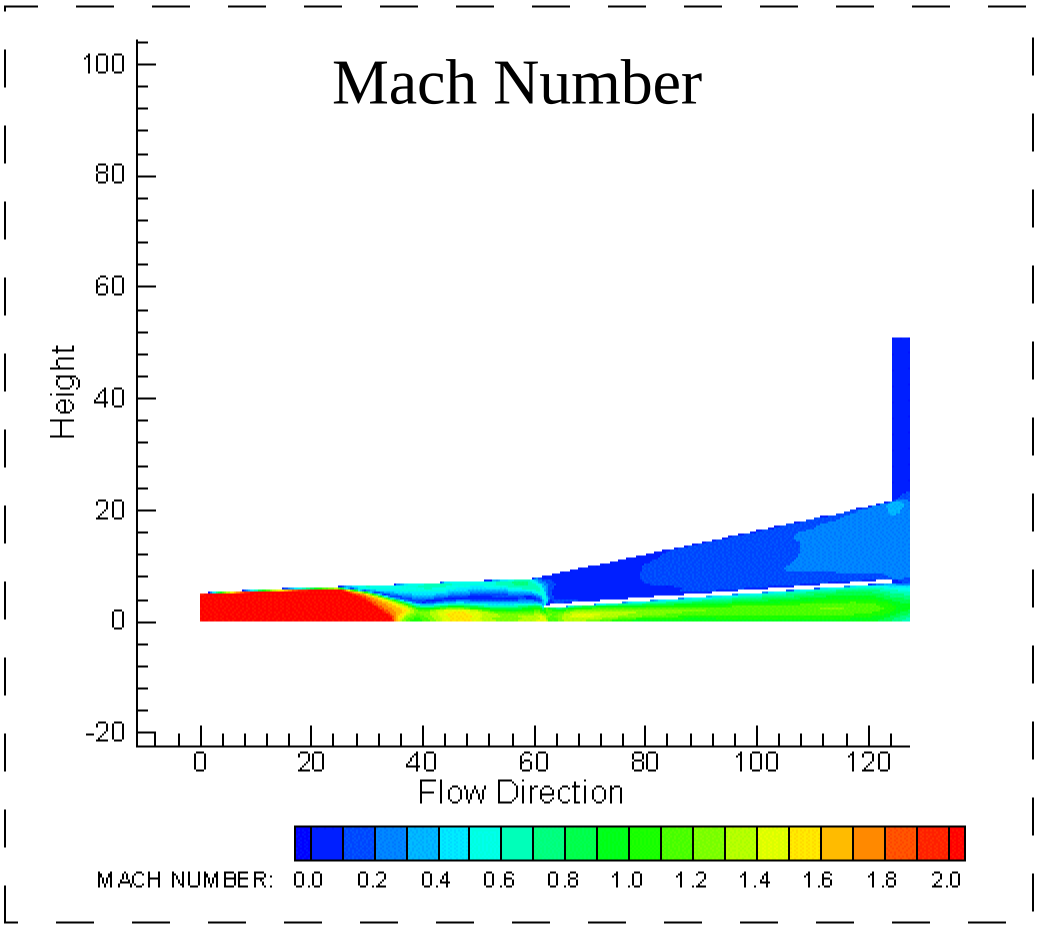
9.98E-06
8.33E-06
6.69E-06
5.04E-06
3.40E-06
1.75E-06
1.10E-07
ICl Mole Fraction Contours
GASPv3 simulation of the RADICL experiment
at P_t = 75 torr.

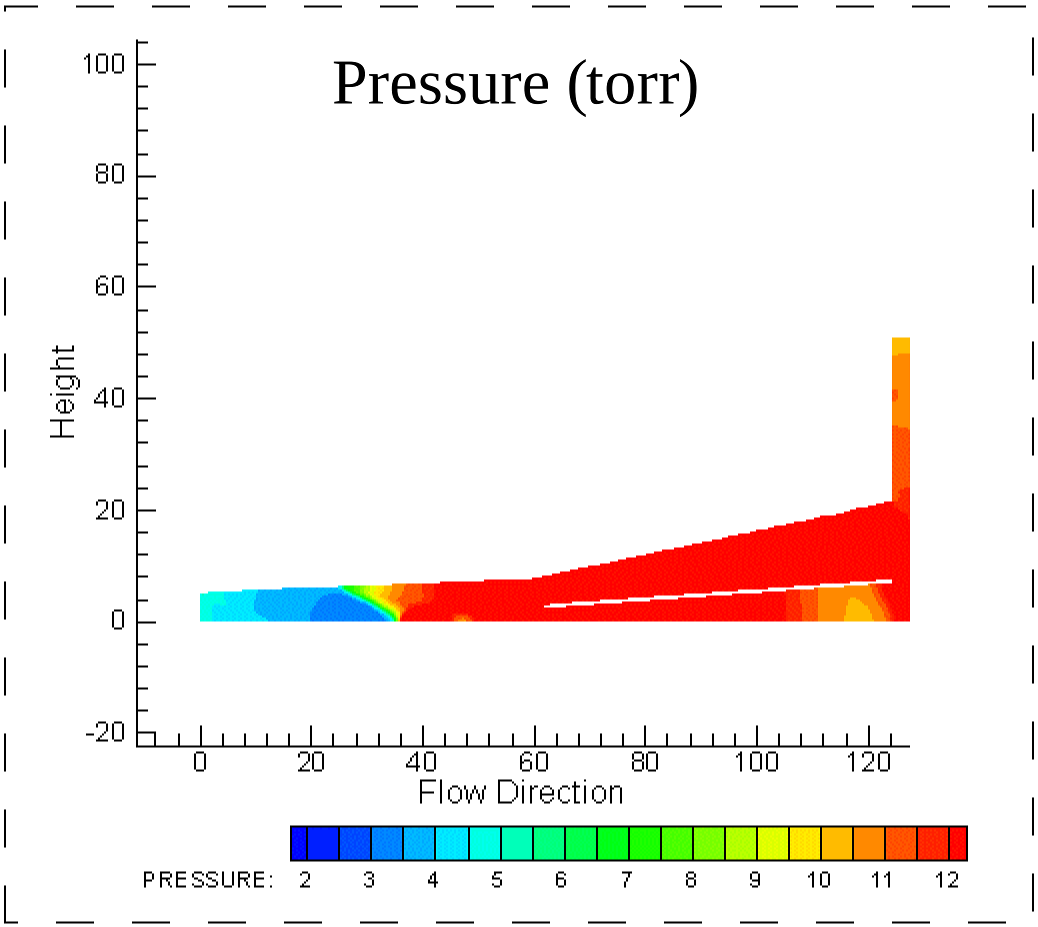
ABL FLM Diffuser



2-D MINT Simulation of the ABL FLM Supersonic Diffuser

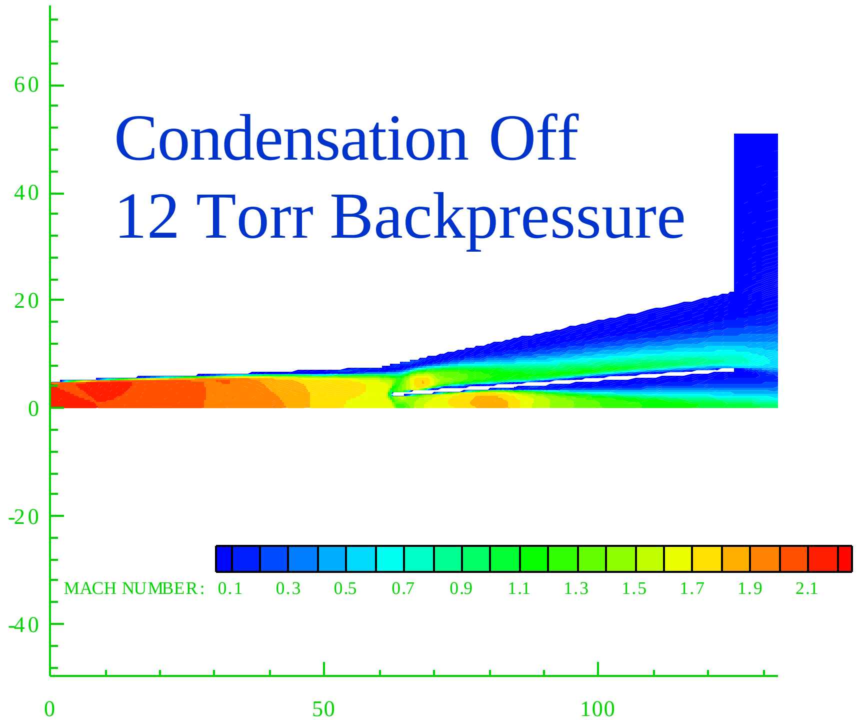


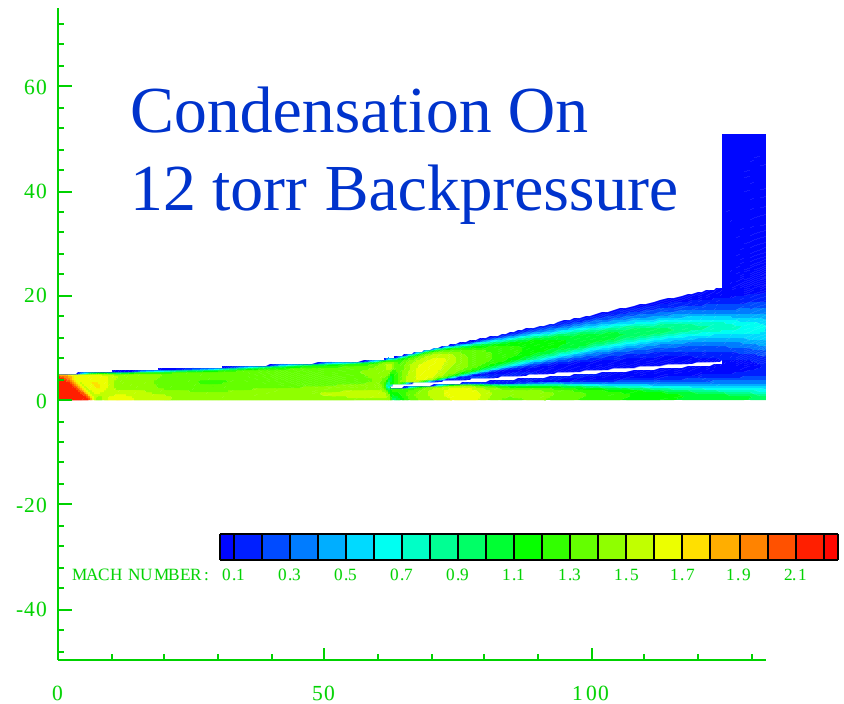
2-D MINT Simulation of the ABL FLM Supersonic Diffuser



2-D MINT Simulation of ABL FLM Diffuser

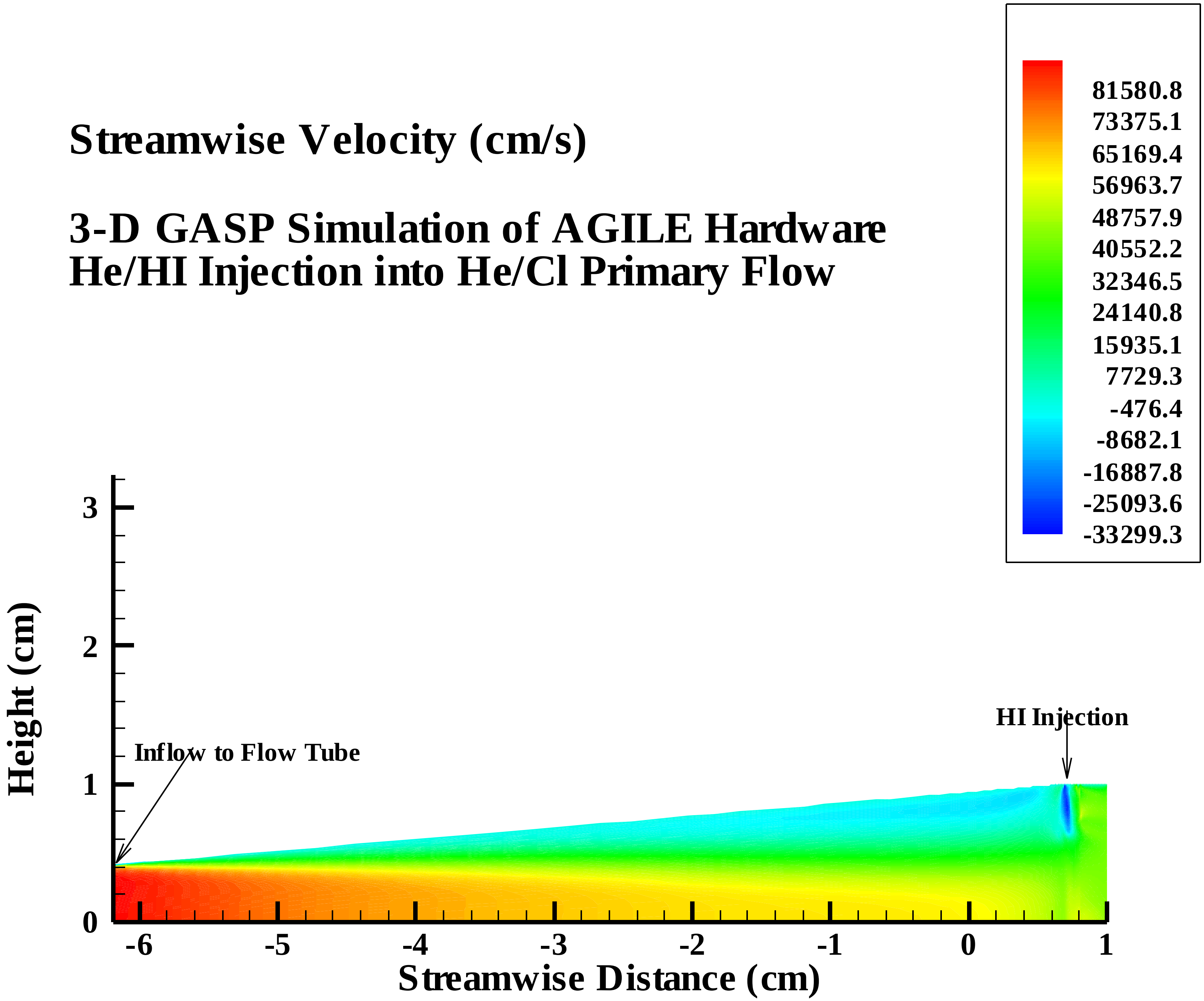
Mach Number





Streamwise Velocity (cm/s)

3-D GASP Simulation of AGILE Hardware He/HI Injection into He/Cl Primary Flow



Challenge Progress to Date

- ABL (with MINT code):
  - 8 2-D FLM diffuser simulations at 4 separate back pressures, with and without H_2O condensation
  - 4 3-D FLM diffuser simulations in progress at 4 separate back pressures.
- RADICL experiment (with GASP):
  - 3-D with reduced 21 reaction, 10 species finite-rate chemistry model, original thermo-chemical database, 3 separate grid resolutions.
  - 3-D with reduced 21 reaction, 10 species finite-rate chemistry model, improved property fits in thermo-chemical database , 2 separate grid resolutions.
  - 3-D with full 45 reaction, 16 species finite-rate chemistry model, improved property fits in thermo-chemical database, 3 separate grid resolutions.

Challenge Progress to Date

- AGIL experiment simulations:
  - 3-D simulation of He/HI injection into He/Cl flow, 1 reaction, 5 species finite rate chemistry, single grid resolution.
  - 3-D simulation of He/HI injection into He/Cl flow, 1 reaction, 5 species finite rate chemistry, new AGIL hardware, in progress.
  - 3-D simulation of He/HN_3 injection into He/Cl flow, 3 reactions, 7 species finite rate chemistry, new AGIL hardware, in progress.

Future Challenge Work

- Develop ‘end-to-end’ 3-D model for ABL FLM.
  - Simulation will include mixing nozzle region, cavity, and diffuser.
  - Will be baselined and validated against existing FLM test data.
  - Will be used to fill in FLM test database with information not measured in tests.
  - Will be used to predict device performance for conditions outside of the parameter space explored in FLM tests.
- Perform 3-D simulations of advanced COIL concepts.
  - Simulate supersonic injection and ‘self-pumped’ mixing nozzle concepts.
  - Results will be placed in ‘end-to-end’ model for prediction of full-scale hardware performance.

Future Challenge Work

- Perform 3-D simulations of AFRL/DELC AGIL experiment hardware.
  - Impact design of upcoming ‘low power’ subsonic device experiments.
  - Evaluate parameter space for future ‘high power’ supersonic device experiments.
- Perform 3-D simulations of AFRL/DELC HF/DF hardware.
  - Support effort to develop understanding of the coupling between fluid dynamics, mixing, and chemistry in the HF/DF chemical laser.
  - Will impact ongoing Space Based Laser (SBL) development work.

Summary

- AFRL/DELC uses 3-D CFD models to simulate the non-equilibrium, chemically reacting, photon emitting gas flow in chemical lasers.
  - The core CFD models are coupled to additional models for the chemical laser physics:
    - » Finite-rate chemistry models.
    - » Conservative, multi-component diffusion model.
    - » Ray trace geometric optics model for near infrared laser radiation field.
    - » H_2O nucleation coupled to Lagrangian particle tracking.

Summary

- Challenge resources have been utilized to provide multiple 2-D and 3-D simulations to date:
  - ABL FLM diffuser simulations:
    - » Effectively demonstrate the influence of H_2O condensation on the diffuser flow field.
  - RADICL experiment simulations:
    - » Identify rate processes that need to be re-measured in experiments.
      - Results will enhance the fidelity of ABL simulations.
  - AGIL experiment simulations:
    - » Identified injectant penetration as possible explanation for mixing issues in experiment hardware.
    - » Identified the presence of a recirculation bubble that would act as a sink for Cl atoms.

Summary

- These Challenge simulations have already impacted ABL and AFRL/DELC programs.
  - Influenced the understanding of the ABL hardware.
    - » This information will affect the design and operating conditions of future hardware.
  - Influencing the design of upcoming AFRL/DELC AGIL experiments.
- Future work will increase the ability of the Challenge simulations to impact these programs.